Supporting Data for the following article published in the ACS journal Biochemistry in 2017:

A fragment profiling approach to inhibitors of the orphan *M. tuberculosis* P450 CYP144A1

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This submission contains the following data:

(1) UV-vis absorbance spectra from the optical titration of CYP144A1 with compound 1, 2, and 4. Protein free spectra has already been subtracted to account for small molecule absorbance. Data are presented as difference spectra (the absorbance of ligand-free CYP144A1 has been subtracted from all spectra). Data are stored as .csv files.

- Titration CYP144 Compound 1_difference spectra
- Titration CYP144 Compound 2_difference spectra
- Titration CYP144 Compound 4_difference spectra

(2) Isothermal titration calorimetry data for the titration of CYP144A1 with compound 3, or the titration of compound 3 into buffer. Data are stored as .csv files.

- ITC Buffer Titration_Compound 3
- ITC Compound 3 Titration

(3) Bioinformatics data from SiteMap and PDBeFOLD analyses of CYP144A1 and CYP121A1 X-ray crystal structures. Data are stored as PDFs

- Site Map Analysis CYP144A1
- PDBeFOLD Analysis

(4) X-band electron paramagnetic resonance spectra for CYP144A1: ligand free, and in complex with compounds 1-5 and with clotrimazole

- EPR_CYP144A1_Compounds 1-3
- EPR_CYP144A1_Fragments 4 5 clotrimazole

(5) Raw fragment profiling data for the unbiased library that was screened by NMR and heme-focused fragment library, which was screened by UV-vis. Data is presented as binary hit (1), non-binding (0). Data are stored as .csv files. SMILES strings for fragments have been provided.

- Fragment profiling_NMR
- Heme focused fragment library_UV-vis

(6) Structural files from the docking of compounds 1-3 into the ligand-freee X-ray crystal structure of CYP144A1. Data are stored as .pdb files.

- Compound 1_Hbonding
- Compound 2_MetalBind_cdx
- Compound 3_water